2,3,4-Trimethylpentane

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.53

Global applicability domain: Inside

Local applicability domain index: 5.39e-01

Confidence level: 6.40e-01

Nearest Neighbors from the Training Set

Image not found
2,4,4-Trimethyl-1-pentene
Measured: 4.55
Predicted: 4.33

Image not found
tert-Butylcyclohexane
Measured: 5.04
Predicted: 5.01

Image not found
Di-tert-butyl ketone
Measured: 3.00
Predicted: 3.20

Image not found
2,2,5,5-
Tetramethyltetrahydrofuran
Measured: 2.06
Predicted: 2.23

Image not found
1,8-Cineol
Measured: 2.74
Predicted: 2.92